Notes on a numerical solver for the Hartree-Fock equation of state of a homogeneous Bose gas

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Intro

As reported in Giorgini's notes [1], the thermodymanics of an homogenous gas of interacting bosons can be obtained analytically in a mean field approximation from the hamiltonian

$$H_{HF} - \mu N = -gnN - \frac{gn_0 N_0}{2} + \sum_k (\epsilon_k - \mu + 2gn)\, a_k^\dagger a_k \tag{1}$$

The equation of state is

Non-condensed phase

$$\begin{cases} n = \dfrac{1}{\lambda_T^3}\, g_{3/2}(e^{\beta(\mu-2gn)}) \\ p = gn^2 + \dfrac{k_B T}{\lambda_T^3}\, g_{5/2}(e^{\beta(\mu-2gn)}) \end{cases} \tag{2}$$

Condensed phase

$$\begin{cases} n = n_0 + \dfrac{1}{\lambda_T^3}\, g_{3/2}(e^{\beta(\mu-2gn)}) \\ \mu = 2gn - gn_0 \\ p = gn^2 - \dfrac{1}{2} gn_0^2 + \dfrac{k_B T}{\lambda_T^3}\, g_{5/2}(e^{\beta(\mu-2gn)}) \end{cases} \tag{3}$$

Numerical solver

We're looking for a tool [2] that solves the equations and gives us the density and the condensed fraction as a function of μ and T, which are the parameters driving the equations above. So given μ and T and of course the atomic quantities (m, g, $\hbar$ etc.) we rewrite everything in the rescaled units

$$\begin{cases} x = n\lambda_T^3 \quad x_0 = n_0\lambda_T^3 & \text{density} \\ \alpha = \beta \dfrac{g}{\lambda_T^3} & \text{temperature parameter} \\ \nu = \mu \dfrac{\lambda_T^3}{g} & \text{chemical potential} \end{cases} \tag{4}$$

And the equations for the density will read

Non-condensed phase

$$x = g_{3/2}(e^{\alpha(\nu-2x)}) \tag{5}$$

Condensed phase

$$\begin{cases} x = x_0 + g_{3/2}(e^{\alpha(\nu-2x)}) \\ \nu = 2x - x_0 \end{cases} \tag{6}$$

Let's find a solution for them.

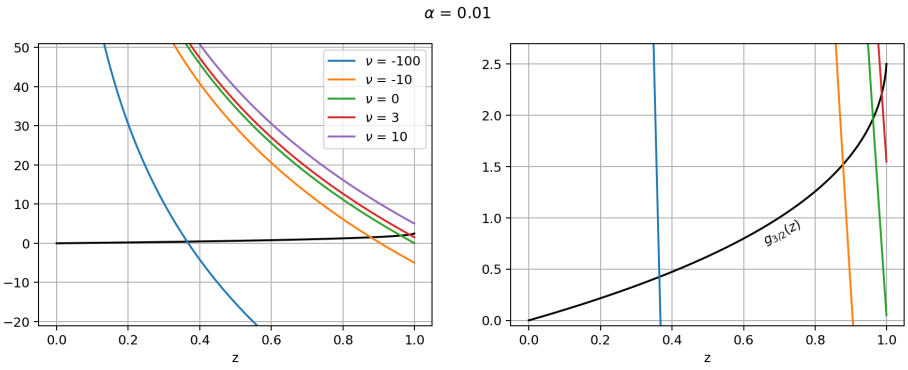

Figure 1: Root finding in the non-condensed phase

Non-condensed phase

Eq. 5 defines implicitly the density of the gas in the case where the condensed fraction is 0. It's useful to change variable to $z = e^{\alpha(\nu-2x)}$, which is the fugacity, substitute for it and numerically find the zero of the function

$$F(z;\alpha,\nu) = g_{3/2}(z) - \frac{\nu}{2} + \frac{1}{2\alpha}\ln z \tag{7}$$

within the domain $z \in [0,1]$.

Given that F is monotonically increasing in z and $F(0) = -\infty$, there exists a unique solution *if and only if* $F(1) = g_{3/2}(1) - \frac{\nu}{2} \geq 0$, that is

$$\nu \leq 2\, g_{3/2}(1) \simeq 5.224 \tag{8}$$

Figure 1 shows an example of solution, plotting $g_{3/2}(z)$ and $x(z) = \frac{\nu}{2} - \frac{1}{2\alpha}\ln z$ for a fixed value of temperature (α), and for different ν. In this phase the total density coincides with the thermal fraction, so from the fugacity we can calculate the non-condensed and condensed densities as

$$\begin{cases} x_t = \dfrac{\nu}{2} - \dfrac{1}{2\alpha}\ln z \\ x_0 = 0 \end{cases} \tag{9}$$

Limited accuracy will affect the result when z is close to its boundaries, that is for z close to 1 (BEC threshold) or for z close to 0 (deep thermal sample). In the latter case, corresponding to a large and negative ν, both the fugacity and the density are expected to be small and one can carry out the following approximations:

$$\nu - 2x \simeq \nu$$
$$g_{3/2}(z) \simeq z$$

resulting in the exponential density of a non interacting classical gas

$$x_t = e^{\alpha\nu} \tag{10}$$

Empirically, this is accurate (within machine precision) well before the numerical solution starts being unstable due to numerical errors, that is for $\nu \leq -10^3$.

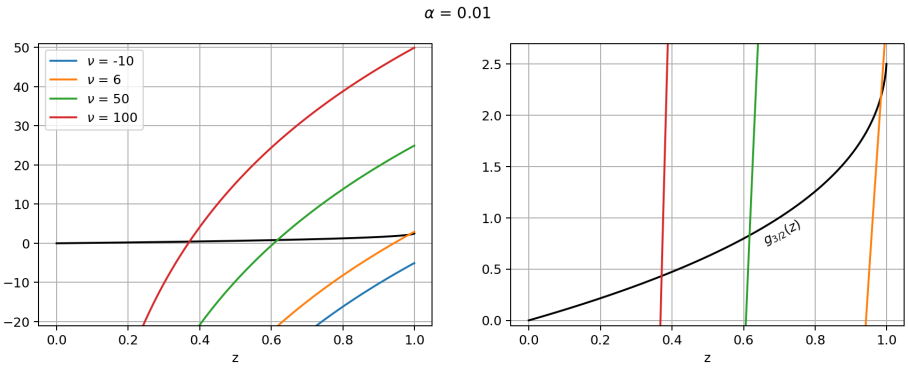

Figure 2: Root finding in the condensed phase

Condensed phase

We use the second of Eq. 6 to eliminate x_0 and make the same substitution for x as a function of the fugacity z, obtaining the function

$$F(z;\alpha,\nu) = g_{3/2}(z) - \frac{\nu}{2} - \frac{1}{2\alpha}\ln z \tag{11}$$

which is almost the same as the previous one, except for a sign change. Now a unique solution always exists provided that $\nu \geq 2g_{3/2}(1)$, which is the correct range of parameters where to use this functional form. An example plot is shown in Fig. 2. Beware that trying to solve this equation in the wrong range can lead to no solution or to two solutions, depending on the value of α, but neither of the two is physically correct.
Calculating the total density x from the solution for z and substituting back in Eq. 6 we get the results for the thermal and condensed densities:

$$\begin{cases} x_t = \dfrac{\nu}{2} + \dfrac{1}{2\alpha}\ln z \\ x_0 = \nu - 2x_t \end{cases} \tag{12}$$

Summary

$$\begin{cases} (\nu \leq 2\,g_{3/2}(1)) \quad F(z) = g_{3/2}(z) - \dfrac{\nu}{2} + \dfrac{1}{2\alpha}\ln z \quad \Rightarrow \quad \begin{cases} x_t = \dfrac{\nu}{2} - \dfrac{1}{2\alpha}\ln z \\ x_0 = 0 \end{cases} \\ (\nu > 2\,g_{3/2}(1)) \quad F(z) = g_{3/2}(z) - \dfrac{\nu}{2} - \dfrac{1}{2\alpha}\ln z \quad \Rightarrow \quad \begin{cases} x_t = \dfrac{\nu}{2} + \dfrac{1}{2\alpha}\ln z \\ x_0 = \nu - 2x_t \end{cases} \end{cases}$$

Figure 3 shows a solution for x_0, x_t close to the transition point.

A bit of physics

Reasonable values

Assuming a sample of Na^{23} atoms, Fig. 4 shows a range of physically plausible values for $\alpha(T)$ and $\nu(\mu, T)$.

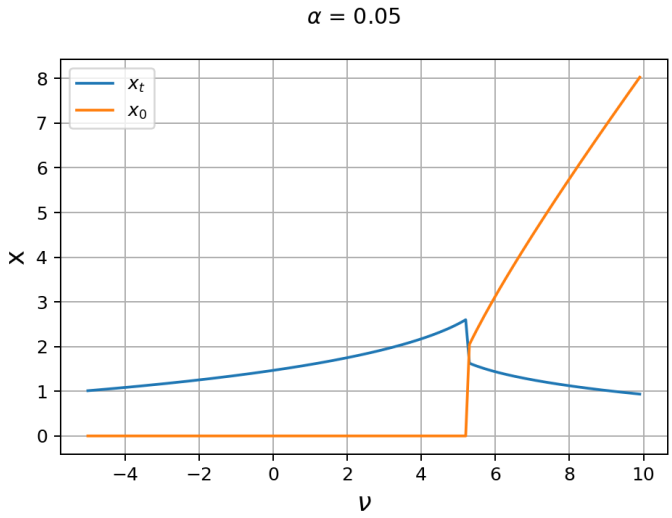

Figure 3: Example solution: thermal and condensed densities vs ν

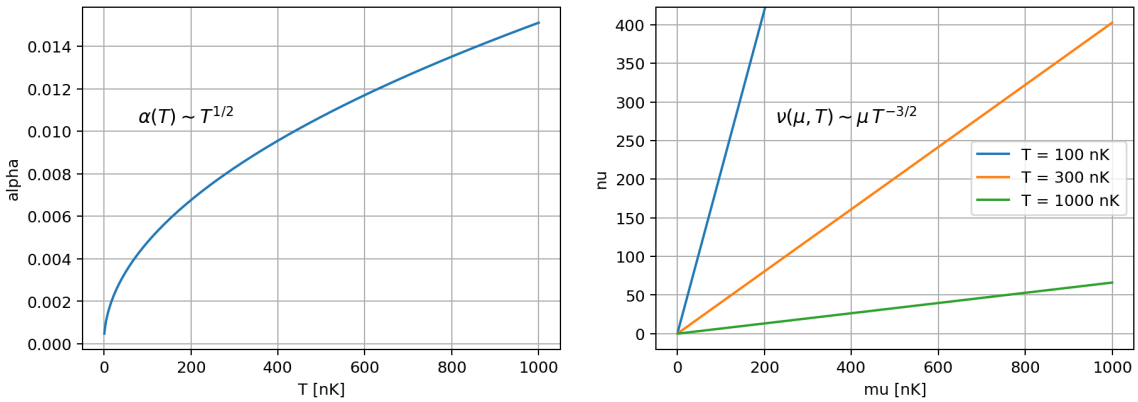

Figure 4: Physical values for $\alpha(T)$, $\nu(\mu, T)$

Harmonic trap

The above equations can be used to predict the density distribution in a inhomogeneous system assuming Local Density Approximation (LDA): in an external potential $V(x)$ one can think each point as being a locally homogeneous sample, whose density is determined by a local chemical potential $\mu(x) = \mu_0 - V(x)$.

Fig. 5 shows the radial density profile of a trapped BEC of Na^{23} atoms, in a spherical harmonic potential with trap frequency $\omega = 2\pi \times 60\,\text{Hz}$, at $T = 300\,\text{nK}$ and $\mu_0 = k_B \times 130\,\text{nK}$. The corresponding adimensional parameters are $\alpha \sim 0.0082$ and ν ranging from 50 in the center to -430 at a radius of 80 µm. This results in a sample of $\sim 6 \times 10^6$ atoms and a BEC fraction $N_0/N \sim 60\,\%$.

References

[1] non lo trovo su internet

[2] https://github.com/carmelom/hfsolver

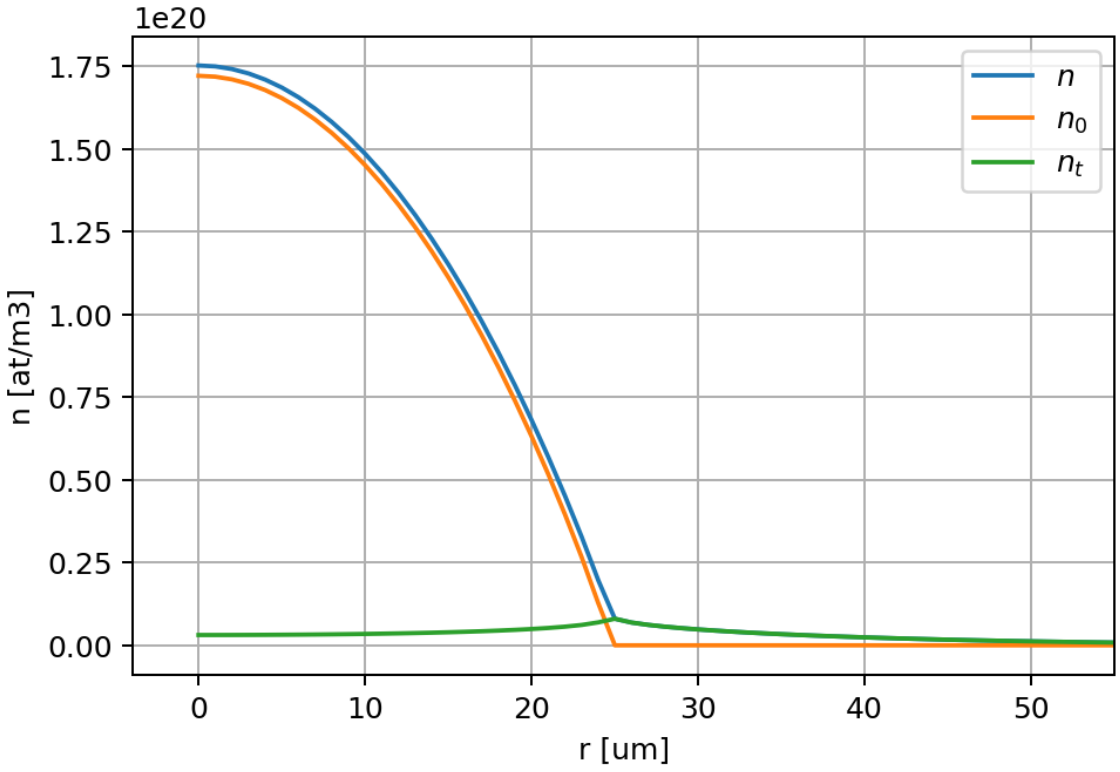

Figure 5: Density of a trapped condensate in a spherical harmonic potential